

Accelerating NLTE radiative transfer by means of the Forth-and-Back Implicit Lambda Iteration: A two-level atom line formation in 2D Cartesian coordinates

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Abstract

State-of-the-art methods in multidimensional NLTE radiative transfer are based on the use of local approximate lambda operator within either Jacobi or Gauss-Seidel iterative schemes. Here we propose another approach to the solution of 2D NLTE RT problems, Forth-and-Back Implicit Lambda Iteration (FBILI), developed earlier for 1D geometry. In order to present the method and examine its convergence properties we use the well-known instance of the two-level atom line formation with complete frequency redistribution. In the formal solution of the RT equation we employ short characteristics with two-point algorithm. Using an implicit representation of the source function in the computation of specific intensities, we compute and store the coefficients of the linear relations $J = a + bS$ between the mean intensity J and the corresponding source function S . The use of iteration factors in the 'local' coefficients of these implicit relations in two 'inward' directions, along with the update of the source function in other two, 'outward', directions leads to four times faster solution than the Jacobi's one. Moreover, the update made in all four consecutive sweeps of the grid leads to an acceleration by a factor of 6-7 compared to the Jacobi iterative scheme.

Keywords: radiative transfer; line formation; numerical techniques

1. Introduction

Radiative transfer (RT) is at the heart of many astrophysical problems. In order to interpret the observed spectra of astrophysical objects it is essential to solve the RT problem. Radiation not only carries the information on the physical state of the medium but also determines its structure and properties. Above all, it plays a fundamental role in the energy and force balance within the medium. Hence the need to take it into account in modern 3D (magneto)hydrodynamic simulations (see, e.g. Hayek et al., 2010). NLTE RT problems are very demanding because of their non-local nature: radiation is decoupled from the *local* thermal state of the gas via scattering processes, so that the state of the gas at one point in the medium depends, via radiative processes, on the state of the gas at all other points. In order to compute emergent intensity in spectral lines (or, in general, the whole set of Stokes coefficients) from a given atmospheric model (with a given run of temperature and pressure/density), the cou-

pled equations of radiative transfer and statistical equilibrium have to be solved. The coupling of the atomic level populations and the radiation fields in the corresponding spectral line transitions is generally highly non-linear. Because of all that, the specific intensity of radiation, which fully describes the radiation field, is a function of seven variables: three spatial and two angular coordinates, frequency and time. Even if we neglect the time dependence for the line transfer problems, and if we use a discretization of all the variables with a grid of 100 points for each of them, we have specific intensity characterized by 10^{12} values. Thus, the solution of the RT problem is very time and memory consuming.

Due to these difficulties, NLTE RT problems have usually been restricted to 1D geometry. However, for many objects (e.g. inhomogeneous stellar atmospheres, rotating stars, accretion disks, solar prominences) the plane-parallel or spherically symmetric 1D approximation is inadequate. Although the theoretical formulation of the multidimensional problem does not differ too much from 1D case, the computational cost is increased by many orders of magnitude. The direct solutions involving the inversion of huge matrices are rather costly, while the most

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simple iterative procedure, so-called Λ iteration¹, that solves the problem equations in turn, is usually too slow to be of practical use (for discussion on its convergence properties see, e.g. [Mihalas, 1978](#)). Thus only fast iterative algorithms enable efficient solution of multidimensional NLTE RT problems with the short characteristics (SC) method almost exclusively used for the formal solution. [Mihalas et al. \(1978\)](#) were the first to apply SC technique for the solution of RT in 2D slab geometries by using difference approximation of the second-order differential equations. [Kunasz & Auer \(1988\)](#) developed an algorithm for the formal solution based on SC solution of the first order differential RT equations and parabolic approximation of the source function. This SC technique was widely exploited in the last three decades within so-called ALI (Accelerated Lambda Iteration) methods, based on the operator perturbation technique (for a review see [Hubeny, 2003](#)). Probably the most commonly used ALI method is Jacobi iteration scheme that employs the diagonal (local) part of the exact Λ operator as an approximate lambda operator (ALO) and computes the error caused by this approximation iteratively ([Olson et al., 1986](#)). It has been extended to NLTE line transfer in 2D (see e.g. [Kunasz & Olson, 1988](#); [Auer & Paletou, 1994](#); [van Noort et al., 2002](#)), and to polarized line RT: in 1D ([Faurobert-Scholl et al., 1997](#)), in 2D cylindrical geometry ([Milić, 2013](#)), and in 3D with partial frequency redistribution (PRD) taken into account ([Anusha & Nagendra, 2011](#)). The convergence rate of the Jacobi method was usually increased by the Ng acceleration technique ([Ng, 1974](#)). The Gauss-Seidel method is twice as fast as the Jacobi method, being usually further accelerated by successive overrelaxation (SOR) technique ([Trujillo Bueno & Fabiani Bendicho, 1995](#)). It was generalized to the 2D line transfer problem by [Léger et al. \(2007\)](#). Another very fast approach is bi-conjugate gradient method (e.g. [Papkalla, 1995](#)) that has been recently generalized to multidimensional polarized line transfer with PRD by [Anusha et al. \(2011\)](#).

Here we propose another approach to the solution of 2D NLTE radiative transfer problems. Our aim is to generalize to 2D geometry the Forth-and-Back Implicit Lambda Iteration - FBILI, previously developed for NLTE line transfer problems in 1D in the paper by [Atanacković-Vukmanović et al. \(1997\)](#), hereinafter ACS97. For simplicity, in this paper we shall use two-level atom model. The multilevel atom case in 1D is considered by ACS97 and the transition from 1D to 2D will be described in a forthcoming paper. FBILI is an extremely fast method, which without additional acceleration technique significantly outperforms available methods in 1D problems (for its convergent properties and the problems solved, see [Atanacković-Vukmanović, 2007](#)). A very fast convergence to the exact solution is achieved by the iterative computation of the coefficients of implicit linear relations between the in-going

radiation field intensities and the line source function during the forward sweep of the 1D grid and by their use in updating the source function together with the specific intensities during the backward sweep. Moreover, the use of an iteration factor in the "local" coefficient of the implicit linear relations enormously increases the convergence rate (for details see Section 2).

We recall the basic idea of FBILI method in the solution of NLTE line formation in 1D geometry in Section 2. The implementation of FBILI method to 2D Cartesian geometry is described in Section 3. In Section 4 we solve a simple test problem and discuss the results, and in Section 5 we comment on our future work.

2. Forth-and-Back Implicit Lambda Iteration (FBILI) basics

The FBILI method is developed and fully described in the paper by ACS97. The essential features of this approach are the following:

- Two-point boundary nature of the problem, i.e. the existence of two separate families of boundary conditions naturally suggests the separate description of the propagation of the in-going intensities of the radiation field $I_{\nu\mu}^-$ with initial conditions at the surface and that of the out-going intensities $I_{\nu\mu}^+$ with initial conditions at the bottom of the system. This recalls the basic idea of a forth-and-back scheme.
- The physics of radiative transfer is almost linear, hence a linear algorithm is feasible for the solution of the problem.
- An implicit representation of the source function is used in the computation of both the in-going and the out-going intensities with a piecewise parabolic behavior of the source function as a suitable assumption.

Before we present the FBILI algorithm in more detail let us stress here the main reason for its high convergence. Slow convergence of the classical Lambda iteration is due to the fact that it computes the *total* mean intensity $J(\tau)$ from the old source function $S^o(\tau)$, keeping thus from the previous iteration more information than necessary. On the contrary, apart from the two-stream representation of the radiation field, in FBILI $J(\tau)$ is split into a local and non-local component, with the local part linearly dependent on the unknown local values of the source function $S(\tau)$ and its derivative $S'(\tau)$. Only the non-local part of the in-going mean intensity $J^-(\tau)$ is computed from the old values $S^o(\tau)$ in the forward step, whereas the non-local part of $J^+(\tau)$ and the local part of both $J^-(\tau)$ and $J^+(\tau)$ are computed from the updated values of $S(\tau)$ in the backward step. The fact that the only piece of information transferred from the previous iteration is contained in the non-local part of the in-going mean intensity $J^-(\tau)$

¹ Λ operator was firstly introduced by Schwarzschild as the operator acting on the source function to give the mean intensity.

enables an extremely high convergence rate of the FBILI method.

In order to demonstrate FBILI approach, we shall consider the two-level atom line transfer with complete frequency redistribution in a static and isothermal plane-parallel 1D medium with no background continuum. Under these assumptions, the RT equation takes the form:

$$\mu \frac{dI_{\nu\mu}(\tau)}{d\tau} = \phi_\nu [I_{\nu\mu}(\tau) - S(\tau)], \quad (1)$$

where $I_{\nu,\mu}(\tau)$ is the specific intensity of the radiation field at the mean optical depth τ , at frequency ν and direction μ (μ is the cosine of the angle between the photon's direction and the outward normal). The absorption-line profile, ϕ_ν , is normalized to unity. The frequency independent line source function is

$$S(\tau) = \varepsilon B + (1 - \varepsilon)J(\tau), \quad (2)$$

where ε is the photon destruction probability, B is the Planck function, and

$$J(\tau) = \frac{1}{2} \int_{-\infty}^{\infty} \phi_\nu d\nu \int_{-1}^1 I_{\nu\mu}(\tau) d\mu \quad (3)$$

is the scattering integral.

The specific intensities incident onto the boundaries, the in-going intensities $I_{\nu\mu}^-(\tau = 0)$ incident onto the surface and the out-going intensities $I_{\nu\mu}^+(\tau = T)$ incident onto the bottom of the medium, are considered given.

In the numerical solution of the RT equation (1) one considers the discrete set of specific intensities with frequencies ν_i , $i = 1, NF$ and directions μ_j , $j = 1, ND$, and evaluates all the relevant depth-dependent functions on a finite grid of mean optical depth values τ_l , $l = 1, NL$.

The propagation of the unknown radiation field "along a ray" can be represented by using the integral form of the RT equation

$$I_{\nu\mu}(\tau_l) = I_{\nu\mu}(\tau_{l-1})e^{-\Delta} + \int_0^\Delta S(t)e^{t-\Delta}dt, \quad (4)$$

and adopting a polynomial representation for the source function $S(\tau)$ between two successive depth points $l-1$ and l . Here, $\Delta = \Delta\tau\phi_\nu/\mu$ is the monochromatic optical path between the two points, with $\Delta\tau = \tau_l - \tau_{l-1}$.

Assuming a piecewise parabolic behavior for the source function we can rewrite the RT equation (4) for the in-going intensities in the following form:

$$I_l^- = I_{l-1}^- e^{-\Delta} + q_l^- S_{l-1} + p_l^- S_l + r_l^- S'_l. \quad (5)$$

Thus we get an implicit linear relation between the in-going specific intensities and yet unknown local source function S_l and its derivative S'_l . For brevity, in Eq. 5 we omitted the dependence of I on ν and μ , and we put the depth index as the subscript of all depth-dependent quantities.

The coefficients p_l^- , q_l^- and r_l^- depend only on the optical distance Δ . The first two terms on the right-hand side of Eq. 5 represent the non-local part of the in-going specific intensity, which is the only one that depends linearly on the old values of the source function at all optical depths $\tau < \tau_l$. The explicit values of I_{l-1}^- are obtained by previous recursive application of Eq. 5 with the old values of $S(\tau)$ and $S'(\tau)$ at $\tau < \tau_l$.

Integrating Eq. 5 over frequencies and directions, we get a local implicit linear relation:

$$J_l^- = a_l^- + b_l^- S_l + c_l^- S'_l. \quad (6)$$

Proceeding from the given upper boundary condition for the in-going intensities at the surface, I_1^- (usually taken to be zero), we compute the coefficients a_l^- , b_l^- and c_l^- at all subsequent depth points $l > 1$ to the bottom, and store them for further use in the backward process of computation of the new values of $S(\tau)$.

In the backward process, using the integral form of the RT equation for the out-going intensities we can write

$$I_l^+ = I_{l+1}^+ e^{-\Delta} + \int_0^\Delta S(t)e^{t-\Delta}dt = I_{l+1}^+ e^{-\Delta} + q_l^+ S_{l+1} + p_l^+ S_l + r_l^+ S'_{l+1}. \quad (7)$$

Here again we assume piecewise parabolic behavior of the source function within each layer (τ_l, τ_{l+1}) .

We start from the bottom layer where the out-going specific intensities I_{NL}^+ are given, and consequently J_{NL}^+ is also known.

By taking into account Eq. 6 for J_{NL}^- , we derive a similar relation for J_{NL} , from which, after we have eliminated the derivative S'_{NL} according to

$$S'_{NL-1} = S'_{NL} = [S_{NL} - S_{NL-1}]/\Delta\tau, \quad (8)$$

we obtain the coefficients a_{NL} , b_{NL} and c_{NL} of the linear relationship

$$J_{NL} = a_{NL} + b_{NL} S_{NL} + c_{NL} S_{NL-1}. \quad (9)$$

On the other hand, Eq. 6 and angle- and line frequency integrated Eq. 7, applied to the point $l = NL - 1$, together with Eq. 8 allow us to express J_{NL-1} also as a linear combination of S_{NL} and S_{NL-1} with the known coefficients:

$$J_{NL-1} = a_{NL-1} + b_{NL-1} S_{NL} + c_{NL-1} S_{NL-1}. \quad (10)$$

Substituting Eqs. 9 and 10 into Eq. 2 for τ_{NL} and τ_{NL-1} , respectively, we can easily derive the new values of S_{NL} and S_{NL-1} . The derivatives S'_{NL} and S'_{NL-1} are obtained from Eq. 8, and the out-going intensities I_{NL-1}^+ from Eq. 7.

Let us note that when we solve RT problem in a constant property, semi-infinite medium (as usual test problem), we take that $J_{NL}^+ = S_{NL}$ and $S'_{NL} = 0$, hence immediately updating the source function according to:

$$S_{NL} = \frac{\varepsilon B + (1 - \varepsilon)a_{NL}^-}{1 - (1 - \varepsilon)(b_{NL}^- + 1)}. \quad (11)$$

For each successive upper depth point we proceed as follows. The coefficients of the relation for J_l^- (Eq. 6) are known from the forward process. Since we assume parabolic behavior of the source function, we can use the relation

$$S'_l = \frac{2}{\Delta\tau}[S_{l+1} - S_l] - S'_{l+1}, \quad (12)$$

to express S'_l in terms of the known values of S_{l+1} and S'_{l+1} and the thus far unknown S_l . Using Eq. 12 we can eliminate the derivative S'_l from Eq. 6 to get J_l^- as a linear function of S_l only. Integrating the formal solution for I_l^+ (Eq. 7) and taking into account that all the terms except S_l are known, similar expression for J_l^+ is straightforwardly derived. Consequently, for each depth point τ_l we obtain the linear relation

$$J(\tau) = a + bS(\tau) \quad (13)$$

that, together with Eq. 2, allows us to derive new value of S_l . With new source function S_l we can compute new derivative S'_l using Eq. 12 and I_l^+ using Eq. 7. So, the computation of the new source function together with the outgoing intensities is performed during the backward process layer by layer to the surface.

Let us stress here that the iterative computation of the coefficients of the implicit relations rather than that of the intensities themselves, provides a high convergence rate. A much higher convergence rate is achieved by the use of the iteration factor $(I_{l-1}^- e^{-\Delta} + q_l^- S_{l-1})/S_l^o$ in the "local" coefficient (coefficient of the local source function S_l) of Eq. 5:

$$I_l^- = \left(\frac{I_{l-1}^- e^{-\Delta} + q_l^- S_{l-1}}{S_l^o} + p_l^- \right) S_l + r_l^- S'_l. \quad (14)$$

In other words, during the forward process at each depth τ_l we retain, for further use in the back-substitution, the ratio of the non-local part of the in-going intensity to the value of the current local source function S_l^o . It represents the only piece of information transferred from the previous iteration. This ratio of two homologous quantities is a good quasi-invariant iteration factor, which plays a very important role in accelerating the iterative procedure. It quickly attains its exact value and leads to the exact solution of the whole procedure with an extremely high convergence rate.

3. FBILI method in 2D

In this Section we shall describe how FBILI method can be implemented in the case of 2D medium in Cartesian geometry.

For simplicity we shall consider again two-level atom line transfer with complete frequency redistribution in a static isothermal medium with no background continuum. Let us assume that the medium is infinite and homogeneous in the z -direction, so that we solve the RT equation in the (x, y) plane (see Fig. 1) in the 'along the ray' form:

$$\frac{dI(x, y, \theta, \varphi, \nu)}{d\tau_s} = \phi(\nu)[I(x, y, \theta, \varphi, \nu) - S(x, y)]. \quad (15)$$

It is assumed that the object is represented by a 2D irregular rectangular grid with NX points in the x -direction and NY points in the y -direction. The direction of propagation of the photons is given by the polar angle θ , measured with respect to the z -axis, and the azimuthal angle φ , measured with respect to the x -axis. The normalized line absorption profile $\phi(\nu)$ for pure Doppler-broadening is given by the Gaussian profile function $\phi(\nu) = \frac{1}{\sqrt{\pi}\Delta\nu_D} e^{-(\nu-\nu_0)^2/\Delta\nu_D^2}$, and $d\tau_s$ is the line integrated optical path length along the ray.

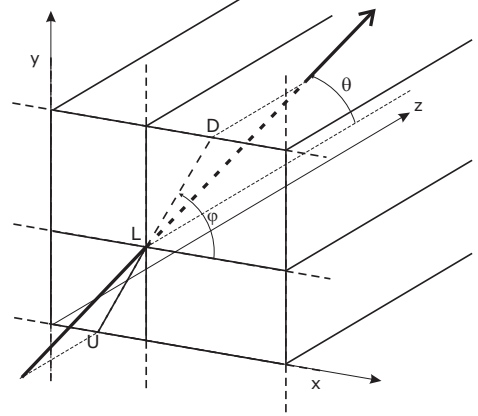


Figure 1: Ray propagation and the definition of angles in 2D geometry. The short characteristics at grid point L for a ray propagating from the lower left intersects the cell boundaries at upwind point U and downwind point D .

The two-level atom line source function in 2D is given by:

$$\begin{aligned} S(x, y) &= \varepsilon B + (1 - \varepsilon)J(x, y) \\ &= \varepsilon B + (1 - \varepsilon)\frac{1}{4\pi} \int_{-\infty}^{\infty} \phi(\nu) d\nu \oint I(x, y, \theta, \varphi, \nu) d\Omega, \end{aligned} \quad (16)$$

where $d\Omega = \sin\theta d\theta d\varphi$.

Here we shall describe how we can solve the problem equations (15) and (16) using the basic ideas of FBILI. Since the formal solution of the RT equation is at the heart of each iterative method we shall first present it as given by ACS97.

3.1. Formal solution

In 2D geometry the formal solution of the RT equation is obtained by sweeping the grid four times. We denote

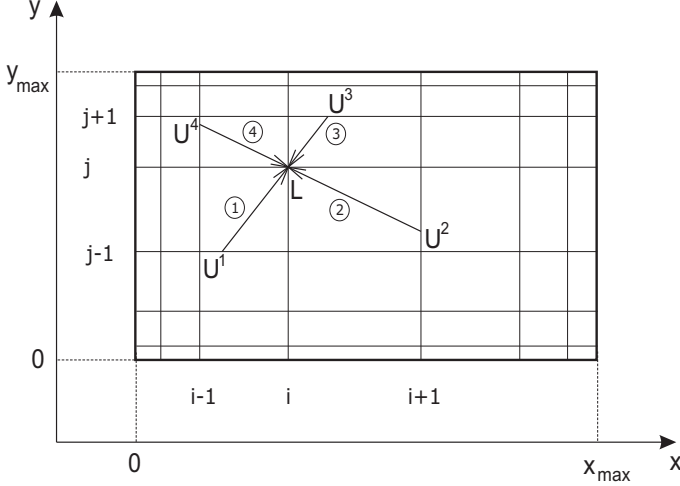


Figure 2: Four sweeps through the local point L of 2D grid in (x, y) plane. Short characteristics and the corresponding upwind points $U^1 - U^4$ are indicated.

by $k (= 1, 2, 3, 4)$ the directions of four sweeps in the corresponding quadrants of the $x - y$ coordinate system (see Fig. 2). Thus 1 denotes the sweep in the direction of increasing x and y , 2 - in the direction of decreasing x and increasing y , 3 - in the direction of decreasing x and y , and 4 - in the direction of increasing x and decreasing y . We take that $y = 0$ is the surface of the medium closer to the observer and we denote the directions 1 and 2 as "inward" and the directions 3 and 4 as the "outward" ones.

Like in most of the contemporary methods, we use the integral form of the radiative transfer equation for its formal solution and the so-called short characteristics approach. In 2D geometry, for each sweep we can rewrite Eq. 4 in the following form:

$$I_L = I_U e^{-\Delta} + \int_0^\Delta S(t) e^{t-\Delta} dt. \quad (17)$$

For simplicity, here we drop index k denoting the sweep because all variables, except $S(\tau)$, are direction (sweep) dependent. Here Δ is the monochromatic optical path between the local grid point $L = (i, j)$ (i.e. point of interest, in which the specific intensity is to be computed) and the "upwind" point U^k , which is the nearest previous intersection point of the direction of propagation of radiation k and the grid lines (see Figs. 1 and 2). The integral in Eq. 17 can be solved analytically if we assume some polynomial representation of the source function on each given subinterval. In the standard short characteristics approach (e.g. Kunasz & Olson, 1988), assuming Lagrangean parabolic approximation, the integral is expressed in terms of the source functions at three points: upwind (U), local (L) and downwind (D) (the latter being the successive intersection point, see Fig. 1), so that Eq. 17 becomes:

$$I_L = I_U e^{-\Delta} + (\Psi_U S_U + \Psi_L S_L + \Psi_D S_D), \quad (18)$$

where the coefficients Ψ follow from the interpolation weights. Instead, for the formal solution FBILI method uses short characteristics at two points, U and L , expressing the integral in terms of the source function at these two points and the source function derivative at local point L :

$$I_L = I_U e^{-\Delta} + p_L S_L + q_L S_U + r_L S'_L. \quad (19)$$

It is important to note that upwind point U is *not* the grid point and that the corresponding values of intensity and source function, I_U and S_U , must be evaluated by interpolation (see e.g. Auer & Paletou, 1994). The coefficients p_L , q_L and r_L depend solely on Δ , and thus implicitly on direction and frequency. If we assume a piecewise parabolic behavior of the source function, their values are easily computed from:

$$\begin{aligned} p_L &= 1 - \frac{2}{\Delta^2} + e^{-\Delta} \left(\frac{2}{\Delta} + \frac{2}{\Delta^2} \right) \\ q_L &= \frac{2}{\Delta^2} - e^{-\Delta} \left(1 + \frac{2}{\Delta} + \frac{2}{\Delta^2} \right) \\ r_L &= -1 + \frac{2}{\Delta} - e^{-\Delta} \left(1 + \frac{2}{\Delta} \right). \end{aligned}$$

Let us note that the specific intensity I and the first derivative of the source function S' are the functions not only of coordinates (like S), but also of direction and frequency. The local derivative of the source function over the optical path length can be expressed in terms of partial derivatives with respect to x and y -axes, and in the case of unit opacity ($\chi = 1$) can be cast into the form:

$$\begin{aligned} S'_L(\nu, \theta, \varphi) &= \frac{1}{\phi(\nu)} \left[\left(\frac{\partial S}{\partial x} \right)_L \cos \varphi \sin \theta \right. \\ &\quad \left. + \left(\frac{\partial S}{\partial y} \right)_L \sin \varphi \sin \theta \right]. \end{aligned} \quad (20)$$

The angles θ and φ are shown in Fig. 1.

Using Eq. 20, Eq. 19 can be written for each sweep as follows:

$$\begin{aligned} I_L &= I_U e^{-\Delta} + p_L S_L + q_L S_U \\ &\quad + r_{L,x} \left(\frac{\partial S}{\partial x} \right)_L + r_{L,y} \left(\frac{\partial S}{\partial y} \right)_L, \end{aligned} \quad (21)$$

where the coefficients $r_{L,x}$ and $r_{L,y}$ follow directly from the above definition of the coefficient r_L and Eq. 20. Once the values of the specific intensity and the source function at the upwind point are obtained by interpolation and after computing the coefficients p_L , q_L , $r_{L,x}$ and $r_{L,y}$, the only values that remain to be computed are the local partial derivatives of the source function with respect to x and y .

3.1.1. Computation of the derivatives

The partial derivatives at the local point are obtained by numerical differentiation. Here we use the Lagrangian

interpolation of the second order in three successive points centered at the local one, that is:

$$\left(\frac{\partial S}{\partial x}\right)_{i,j} = w_{i-1,j,x}S_{i-1,j} + w_{i,j,x}S_{i,j} + w_{i+1,j,x}S_{i+1,j}, \quad (22)$$

and

$$\left(\frac{\partial S}{\partial y}\right)_{i,j} = w_{i,j-1,y}S_{i,j-1} + w_{i,j,y}S_{i,j} + w_{i,j+1,y}S_{i,j+1}. \quad (23)$$

The explicit expressions for the weights in Eq. 22 are:

$$\begin{aligned} w_{i-1,j,x} &= \frac{(x_i - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} \\ w_{i,j,x} &= \frac{1}{x_i - x_{i+1}} + \frac{1}{x_i - x_{i-1}} \\ w_{i+1,j,x} &= \frac{(x_i - x_{i-1})}{(x_{i+1} - x_i)(x_{i+1} - x_{i-1})} \end{aligned} \quad (24)$$

The weights used in Eq. 23 have the same form, except they depend on the discrete values of y . At the boundaries of the grid, linear approximation is used. Let us note that the local source function $S_{i,j}$ contributes to the local partial derivatives, so that its weight can be summed up with the coefficient p_L in Eq. 21. In some iterative procedures described in the next section this led to better stability and the convergence rate of the method.

The formal solution given above will be implemented in various iterative schemes described in the next section.

3.2. Iterative procedures

Let us recall again that the simplest iterative scheme, Λ iteration, computes the mean intensity ($J = \Lambda S$) and the source function ($S = S(J)$) in turn. In order to compute the mean intensity at any grid point it is necessary to perform four sweeps of the grid, i.e. to compute the specific intensities (using Eq. 21) at all previous grid points along each sweep with the old (known from the previous iteration) values of the source function. Once the mean intensities at all grid points are obtained, one can compute new source function using Eq. 16. Iterations are repeated until the convergence is achieved. As already mentioned, this is an extremely slow procedure because it transfers from one part of the iterative step to the other more information than necessary. In what follows we shall explain how Λ iteration in 2D has been accelerated up to now and how it can be further accelerated by our approach. More specifically, we shall describe our implementation of Jacobi and Gauss-Seidel methods, and two variants of the FBILI procedure applied to 2D line transfer problem.

3.2.1. Jacobi-type iteration

An efficient way to accelerate Λ iteration is to simplify the full description of the RT process, i.e. to use an approximate lambda operator (ALO), Λ^* , instead of the full (exact) Λ one, accounting for an error introduced by

this approximation iteratively. Using "operator splitting" (well-known from numerical analysis) in RT computations, the formal solution of the RT equation can be written in the form:

$$J = \Lambda S = (\Lambda - \Lambda^*)S + \Lambda^*S. \quad (25)$$

Olson et al. (1986) were the first to point out that the diagonal of the exact Λ matrix itself represents an almost optimum ALO.

Here, we shall describe the Jacobi-type iterative procedure and see that the coefficient of the local source function b_L plays a role of the diagonal ALO in the Jacobi method.

In the Jacobi-type procedure applied to 2D radiative transfer, first we have to sweep the grid 4 times, and in every sweep k to compute and store the coefficients of the linear relation:

$$J_L^k = a_L^k + b_L^k S_L. \quad (26)$$

This equation is obtained by the angle- and line profile integration of Eq. 21, in such a way that the coefficient a_L^k contains all non-local contributions to the specific intensity at the given point L :

$$\begin{aligned} a_L^k &= \frac{1}{4\pi} \int_{-\infty}^{\infty} \phi(\nu) d\nu \int \left[I_U^k e^{-\Delta^k} + q_L^k S_U^k + \right. \\ &\quad \left. r_{L,x}^k \left(\frac{\partial S}{\partial x}\right)_L^k + r_{L,y}^k \left(\frac{\partial S}{\partial y}\right)_L^k \right] d\Omega, \end{aligned} \quad (27)$$

and is computed using the current values of the source function and its derivatives, whereas the coefficient b_L^k has the form:

$$b_L^k = \frac{1}{4\pi} \int_{-\infty}^{\infty} \phi(\nu) d\nu \int p_L^k d\Omega, \quad (28)$$

playing the role of the diagonal ALO. To be consistent, the contribution of the local source function to the local partial derivatives (see Eqs 22 and 23) should be included in the coefficient b_L^k rather than in the coefficient a_L^k .

The total mean intensity at point L is obtained by summing up mean intensities in all the sweeps, and is given by

$$J_L = a_L + b_L S_L, \quad (29)$$

where $a_L = \sum_{k=1}^4 a_L^k$ and $b_L = \sum_{k=1}^4 b_L^k$ are the total coefficients.

Once we know the coefficients of Eq. 29, by inserting Eq. 29 into Eq. 16 we can update the source function at all depth points throughout the 2D grid by means of:

$$S_L = \frac{\varepsilon B + (1 - \varepsilon) a_L}{1 - (1 - \varepsilon) b_L}. \quad (30)$$

In this way, the iterative computation of the coefficients a_L and b_L of the implicit relation (29) instead of the unknown quantities (J_L and S_L) themselves leads to much

more efficient corrections than in Λ iteration. This scheme reduces number of iterations by a few orders of magnitude with respect to the ordinary Λ iteration. However, even this is not fast enough for some more demanding problems (strong, scattering dominated lines).

3.2.2. Gauss-Seidel-type iteration

As it has just been explained, in the Jacobi iteration the grid is swept four times and in every sweep the coefficients a_L^k and b_L^k are computed from the "old" values of the source function. Only after getting the total coefficients a_L and b_L at all grid points, the source function is updated using Eq. 30.

The Jacobi scheme can be substantially accelerated if the new source function is computed *as soon as the total coefficients a_L and b_L in Eq. 29 are available (known)* at some point. This is, for example, the situation at the boundary grid points after sweeping the grid three times and computing the corresponding coefficients a_L^k and b_L^k ($k = 1, 3$). We start the fourth sweep with given values of a_L^4 and b_L^4 at two boundaries: $(1, j)$; $j = 1, NY$ and (i, NY) ; $i = 1, NX$ (see Fig. 3). The new source function S_L at these points is easily computed using Eq. 30. Now, our aim is to come up with the scheme which will use this idea at all subsequent points as the use of "new" (updated during the current sweep) source functions in the computation of the local intensities in the fourth sweep accelerates the convergence. This numerical scheme corresponds to Gauss-Seidel method known from numerical algebra (see e.g. Saad, 2003). For the solution of the 1D NLTE RT problem this idea was implemented in two different ways by Trujillo Bueno & Fabiani Bendicho (1995) and Atanacković-Vukmanović et al. (1997). In the paper by Trujillo Bueno & Fabiani Bendicho (1995) standard approximate Λ operator approach with three-point algorithm to set up short characteristics of the second order is used. This method has been explicitly generalized to 2D geometry by Léger et al. (2007). The FBILI method, developed by Atanacković-Vukmanović et al. (1997), uses two-point algorithm and computes the coefficients of the implicit relations expressing the intensities in terms of the source functions and its derivatives at pairs of successive depth points.

The whole procedure is more complicated in multidimensional geometries because of the spatial interpolations needed to obtain values of the upwind source function and intensities. Let us consider the procedure in 2D in more detail.

Fig. 3 describes the situation upon arrival at the grid point (i, j) in the last, fourth sweep, after the 2D grid was swept three times. We assume that the source function is already updated in the points represented by full dots. From now on we shall refer to the sweeps during which the formal solution is performed, and appropriate coefficients are stored, with no update of the source function as the *forward* sweeps, whereas the sweeps during which

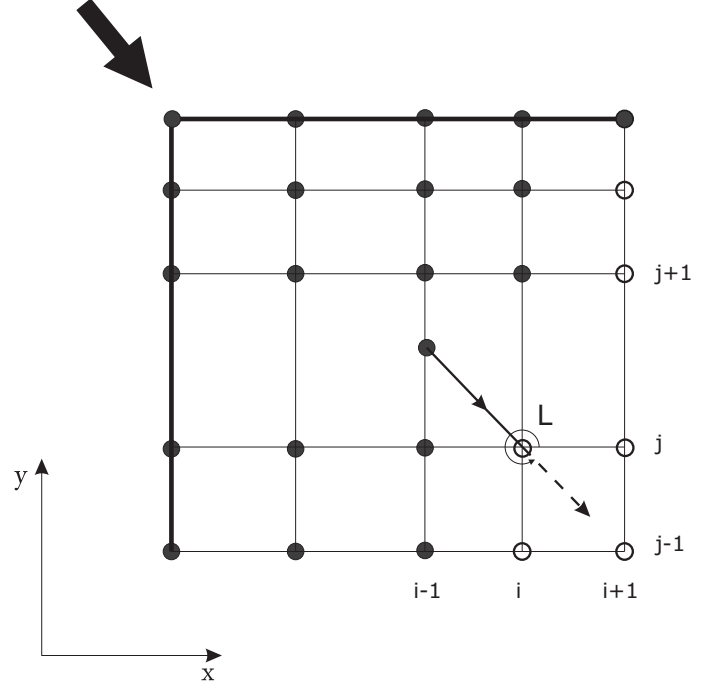


Figure 3: 2D grid sweep in the 4th direction. Full dots correspond to the new values of the source function, empty ones to the old values.

the source function is updated as the *backward* ones ².

It is essential to realize that all the non-local contributions to the coefficient a_L in Eq. 30 must be properly taken into account. Some of these contributions are already updated in the current sweep ("new"), while the others still have their values from the previous iteration ("old").

In our implementation of Gauss-Seidel iterative scheme we first modify the formal solution in the following way: We use Eq. 21 with partial derivatives given by Eqs. 22 and 23, thus expressing explicitly the contributions of $S_{i-1,j}$, $S_{i+1,j}$, $S_{i,j-1}$ and $S_{i,j+1}$ to the local specific intensity. Furthermore, upwind source function S_U is also expressed in terms of the source function values at the neighboring grid points. As an example, for the point U_1 in Fig. 2 we have:

$$S_U = W_{i-1,j-1}S_{i-1,j-1} + W_{i,j-1}S_{i,j-1} + W_{i+1,j-1}S_{i+1,j-1}. \quad (31)$$

In the above equation the weights W follow from the Lagrangean interpolation of the second order, and, for convenience, we give the expressions:

²For example, Jacobi iteration consists of four forward sweeps followed by the simultaneous update of the source function over the entire grid.

$$\begin{aligned}
W_{i-1,j-1} &= \frac{(x_U - x_i)(x_U - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})}, \\
W_{i,j-1} &= \frac{(x_U - x_{i-1})(x_U - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})}, \\
W_{i+1,j-1} &= \frac{(x_U - x_{i-1})(x_U - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}. \quad (32)
\end{aligned}$$

Finally, Eq. (21) for each sweep k takes the new form:

$$I_L^k = I_U^k e^{-\Delta^k} + p_L^k S_L + \sum_{i'} \sum_{j'} r_{i',j'}^k S_{i',j'}. \quad (33)$$

The expression for the parabolic interpolation formula in the above equation is similar to the one given by Eq. 5 in the paper by Kunasz & Auer (1988). Here the coefficients $r_{i',j'}$ follow from the approximations used to compute the local derivative of the source function S_L' and to interpolate the value of the source function at upwind point S_U . Note that $r_{i,j}$ (indices (i,j) refer to the grid point L) is always zero, as all local contributions are added to the coefficient p_L . This way, all non-local contributions (in all sweeps) except the upwind specific intensities are explicitly expressed using eight neighboring source functions.

Integration of Eq. 33 over angles and line profile yields:

$$J_L^k = a_L^k + b_L^k S_L + \sum_{i'} \sum_{j'} c_{i',j'}^k S_{i',j'}. \quad (34)$$

Here, the coefficients are defined as:

$$a_L^k = \int \phi(\nu) d\nu \int \frac{d\Omega}{4\pi} I_U^k e^{-\Delta^k}, \quad (35)$$

$$b_L^k = \int \phi(\nu) d\nu \int \frac{d\Omega}{4\pi} p_L^k, \quad (36)$$

and

$$c_{i',j'}^k = \int \phi(\nu) d\nu \int \frac{d\Omega}{4\pi} r_{i',j'}^k. \quad (37)$$

After computing the coefficients a_L^k , b_L^k and $c_{i',j'}^k$ in all four directions, the source function can be updated according to:

$$S_L = \frac{\varepsilon B + (1 - \varepsilon)(a_L + \sum_{i'} \sum_{j'} c_{i',j'} S_{i',j'})}{1 - (1 - \varepsilon)b_L}, \quad (38)$$

where $a_L = \sum_k a_L^k$, $b_L = \sum_k b_L^k$ and $c_{i',j'} = \sum_k c_{i',j'}^k$.

Let us point out here that the upwind intensity I_U^4 , contained in the coefficient a_L^4 , is computed from the updated source function at previous points along the fourth sweep. It is important to stress that if Eq. 38 is used to update the source function in the backward sweep, all the proper contributions of “new” and “old” neighboring source functions are *automatically* taken into account, through the sum $\sum_{i'} \sum_{j'} c_{i',j'} S_{i',j'}$. We now propose the following, Gauss-Seidel like scheme:

1. Sweep the grid in the first three directions (forward sweeps), computing and storing the corresponding coefficients a_L^k , b_L^k and $c_{i',j'}^k$, ($k = 1, 3$) of Eq. 34 by means of the old values of the source function.
2. Start the fourth (backward) sweep. At the grid points on the two boundaries (marked in bold in Fig. 3), specific intensities of the incident radiation field are known so that a_L^4 , b_L^4 and $c_{i',j'}^4$ are known, and the source function S_L can be straightforwardly computed using Eq. 38. After updating the source function, specific intensity I_L^4 is computed using Eq. 33.
3. At all the subsequent points of the backward sweep, with the updated values of the specific intensities I_L^4 at previous points, the upwind intensity I_U^4 is to be computed, and, hence the coefficient a_L^4 . Once the total coefficients a_L , b_L and $c_{i',j',L}$ are obtained, the source function is updated by means of Eq. 38 and specific intensity is computed using Eq. 33.
4. Steps 1-3 are repeated until convergence.

The main difference between this scheme and the above described Jacobi-like scheme is that the source function is updated *in the course* of the fourth sweep (instead *after* the fourth sweep is completed). This modification introduced by the Gauss-Seidel approach significantly increases the rate of convergence. As we shall see in the next section, even further acceleration in 2D is possible by the application of the forth-and-back approach and the use of iteration factors.

3.2.3. “Two-by-two” FBILI method

FBILI method proposed by ACS97 brought about improvements over the existing ones in the following: (i) iterative computation of the coefficients of the implicit linear relation between the specific intensities and the local source function and its derivative in the forward sweep, combined with an efficient method of back-substitution (a two-point, not a three-point scheme), led to a quick update of S and S' along the 1D grid, and (ii) the use of iteration factor in the forward sweep, which “enhances” the local operator by $(I_U e^{-\Delta} + q S_U)/S_L$, provided an extremely fast convergence with respect to the previous schemes. The acceleration of the iterative procedure is due to the fact that it is much faster to iterate on the ratio of the two unknowns than on the unknowns themselves. In 1D case, introduction of the iteration factor increased the convergence rate of the FBILI method by a factor of 3.

In order to generalize FBILI to 2D we ought to take into account that, due to the twofold two-point boundary nature of the problem, we have two pairs of the mutually opposite sweeping directions (1-3 and 2-4). We can, therefore, emulate the original FBILI approach by considering two inward directions (1 and 2) as the forward ones and two outward directions (3 and 4) as the backward ones. The update of the source function is thus performed twice during the single iteration. Moreover, in the forward

sweeps we can introduce appropriate iteration factors into the 'local' coefficient b_L to speed up the convergence.

In general, the method can be used in many different ways: it is possible to use iteration factors in one or two directions, or not at all; there can be one, two, or even four backward sweeps. In the following we present some of the most efficient schemes.

As before, we use Eqs. 33 and 34, and we include the iteration factors in the computation of the coefficient b_L during the two in-going (forward) sweeps 1 and 2:

$$b_L^{1,2} = \int \phi(\nu) d\nu \int (p_L^{1,2} + \frac{I_U^{1,2} e^{-\Delta^{1,2}}}{S_L^{\text{old}}}) d\Omega, \quad (39)$$

while in the out-going (backward) directions the coefficient b_L contains only direction- and line profile-integrated coefficient p_L from Eq. 33.

We propose the following iteration procedure:

1. Sweep the grid three times (forward sweeps), computing the specific intensity using Eq. 33 and iteration factors in directions 1 and 2 as given by Eq. 39. Compute the corresponding coefficients a_L^{1-3} , b_L^{1-3} and $c_{i',j'}^{1-3}$.
2. In the fourth (backward) sweep, starting from the grid points on two corresponding boundaries with known boundary conditions, update the source function by means of Eq. 38 and the out-going specific intensity using Eq. 33 point by point throughout the grid. Reset coefficient b^1 to zero (as the iteration factor is used, a^1 is zero by default).
3. Sweep the grid in direction 1 (iteration factor is used). Reset a^3 and b^3 to zero.
4. Sweep the grid in direction 3 (no iteration factor). *Update the source function and the intensity while performing the sweep.* Note that this sweep is now backward sweep. Reset b^2 to zero (a^2 is zero by default).
5. Sweep the grid in direction 2 (iteration factor is used). Reset a^4 and b^4 to zero.
6. Sweep the grid in direction 4 (no iteration factor). *Update the source function and the intensity while performing the sweep.* Reset b^1 to zero.
7. Repeat steps 3-6 until convergence.

The only differences in the above scheme, with respect to our GS-like procedure described in section 3.3.2 are: (a) inclusion of factors in "in-going" directions 1 and 2, (b) a re-ordering of directions (for better stability), and (c) updating of the source function in "out-going" directions 3 and 4, i.e. there are two backward sweeps now instead of just one. Hence, the source function is updated twice per iteration, i.e. once per each pair of the mutually opposite sweeping directions (1-3 and 2-4). This implementation shows a very good stability and also much better convergence properties with respect to other methods described previously. This inspired us to try to further accelerate the method by updating the source function *in all four sweeps*.

3.2.4. "Sweep by sweep" FBILI procedure

In the previous section we have seen that the update of the source function can be performed more than once during a single iteration. This idea was realized in 1D plane-parallel geometry by means of SSOR (symmetric successive overrelaxation) method (see, for example: [Sampoorna & Trujillo Bueno, 2010](#)). In principle, as soon as the grid is swept four times in the first iteration and coefficients a^{1-4} , b^{1-4} and $c_{i',j'}^{1-4}$ are known, one can update the source function in *every* sweep of the grid.

Here, the only difference with respect to the "two-by-two" procedure is that after the step 2, source function is updated during all four sweeps ("sweep by sweep"). This leads to four updates per iteration at essentially no additional computational cost (computation of the source function takes negligible time with respect to the formal solution). This very same procedure without iteration factors would correspond to Symmetric Gauss-Seidel (SGS) in 2D geometry. As we shall see in the next section, this method, with the help of iteration factors, extremely accelerates the convergence with no additional numerical acceleration technique.

4. Results

In order to test the properties of the above mentioned procedures we solve the problem given by [Auer & Paletou \(1994\)](#). We consider a slab with optical depth $\tau = 10^4$ along both (x and y) axes, with $\varepsilon = 10^{-4}$, $B = 1$, and Doppler profile. Equidistant logarithmic spacing in optical depth with approximately 10 points per decade (129×129 points) is used. The slab is irradiated at bottom and at side boundaries, from the angles $\pi < \varphi < 2\pi$, with radiation equal to B . For angular integration we use Carlson's set B ([Carlson, 1963](#)) with $n = 8$ (12 angles per octant). We use 9 frequency points in a half of the line profile, and the trapezoid integration weights.

The properties of the iterative procedures are analyzed by calculating at each iteration step i the maximum relative change of the solution between two successive iterations $i - 1$ and i :

$$R_c^i = \left| \frac{S_c^i - S_c^{i-1}}{S_c^i} \right|_{\text{max}}. \quad (40)$$

The first tested procedure, denoted here as Jacobi-type procedure, needed 118 and 195 iterations to reach the maximum relative change $R_c = 10^{-3}$ and $R_c = 10^{-5}$, respectively. From these results it is evident that higher convergence rate is desired. As mentioned before, it is customary to apply Ng acceleration ([Ng, 1974](#)) to Jacobi method. However, since it requires some experimentation (its use is not straightforward), we have not used it, i.e. we present here the results with no additional mathematical acceleration techniques like the Ng's.

When we applied the second, Gauss-Seidel type procedure we obtained the corresponding solutions in 77 and

126 iterations. The increase in the convergence rate is evident, but not as great as in 1D case.

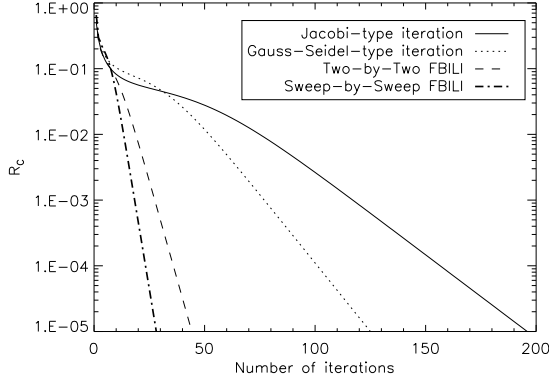


Figure 4: Variation of the maximum relative change with iterations for the iterative procedures considered.

Finally, two FBILI procedures with iteration factors ("2-by-2" and "sweep-by-sweep") dramatically increased the convergence rate (see Fig. 4). In these two procedures, we define one iteration as the whole set of four sweeps, although the source function is updated two(four) times (recall that the computation of the source function is very fast). "Two-by-two" FBILI with iteration factors in directions 1 and 2 reaches $R_c = 10^{-3}$ in 28 iterations and $R_c = 10^{-5}$ in 44 iterations, while the "sweep-by-sweep" procedure with iteration factors in two inward directions and source function update in all four sweeps achieves the above relative changes in 19 and 29 iterations, respectively (6-7 times faster than Jacobi scheme). Omitting the iteration factors in the procedure that updates the solution in all four directions leads to the iterative scheme corresponding to the generalization of the Symmetric-Gauss-Seidel method. Using this procedure the above convergence criteria are satisfied in 39 and 61 iterations, respectively. The importance of the iteration factors is evident, as they improve the convergence rate of SGS by a factor of more than two.

In order to study the performance of an iterative method, also the *true* error ought to be analyzed. Since the analytical solution of this benchmark problem cannot be obtained, the true error is expressed with respect to S_{REF}^{∞} - the fully converged "exact" solution obtained with some well-tested code. In this case we used the 1000th Jacobi iteration, with four times more dense spatial grid (for which $R_c \approx 10^{-15}$) as the "exact" solution. Considering that the source function along the central line of the slab, $S(NX/2, j)$; $j = 1, NY$, has a similar behavior to the solution in a 1D semi-infinite stellar atmosphere, we took central surface point as the point of interest in analyzing the true error. So, we define maximum relative true error as:

$$T_e^i = \left| \frac{S(NX/2, 1)^i - S(NX/2, 1)_{\text{REF}}^{\infty}}{S(NX/2, 1)_{\text{REF}}^{\infty}} \right|_{\text{max}}. \quad (41)$$

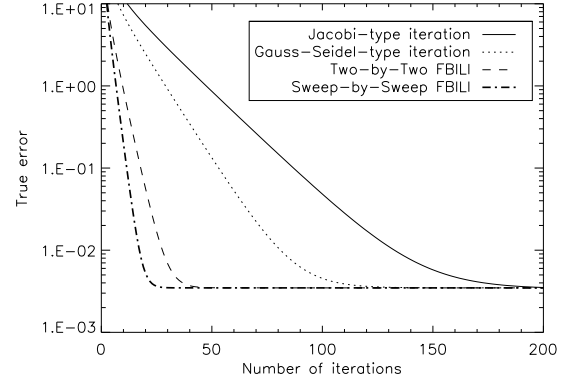


Figure 5: Variation of the true error with iterations for the procedures considered.

Change of the true error with number of iterations is shown in Fig. 5. Excellent properties of FBILI method are again evident. For a fast converging method such as this one, one can actually use weaker convergence criterion in terms of R_c . To make this statement clear, recall that slowly converging method will reach small relative change relatively quickly, but might still be far from the "true" solution. We stress that, in principle, the true error should be the convergence criterion, but as it is not known, good knowledge of the convergence properties of the method in question must be obtained in order to set proper value of R_c as the convergence criterion, thus optimizing the computing time.

5. Conclusions

We have presented main concepts of a new iterative scheme for the NLTE line radiative transfer in 2D Cartesian geometry. Introduction of iteration factors in the 'local' coefficient of the linear relation between J and S , combined with the idea of using new values of the source function as soon as they are available in all four sweeps of the grid dramatically improves the convergence rate.

Even better comparative convergence properties of FBILI method can be expected in applications to some more realistic problems; e.g. in the semi-infinite atmosphere with periodic boundary conditions. Just as 1D FBILI iterative scheme shows its full advantage for optically thick media and scattering dominated problems that need fast methods to be solved efficiently, we aim to achieve the same in the 2D and 3D cases. Our first goal is to implement periodic boundary conditions in the code and also to test more accurate interpolating strategies (for example, cubic interpolation, as suggested by [Simonneau et al., 2012](#)) in

computing formal solution, the source function derivatives, and the spatial interpolation at the upwind point. We also aim to generalize the backward elimination scheme from 1D FBILI to 2D, i.e. to eliminate the local derivative by means of the source function and the derivative at previous grid points. This would eliminate need for keeping eight $c_{i'j'}$ coefficients and lead to more elegant solution.

In the future work we will also test scaling of convergence properties with respect to grid resolution and demonstrate generalization of the method to multilevel atom case, as well as to PRD problems and polarized line transfer in a two-level atom approximation.

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